A simple theory for high Δ/T_c ratio in d-wave superconductors

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We investigate a simple explanation for the high maximum gap to T_c ratio found experimentally in high T_c compounds. We ascribe this observation to the lowering of T_c by boson scattering of electrons between parts of the Fermi surface with opposite sign for the order parameter. We study the simplest possible model within this picture. Our quantitative results show that we can account for experiment for a rather small value of the coupling constant, all the other ingredients of our model being already known to exist in these compounds. A striking implication of this theory is the fairly high value of the critical temperature in the absence of boson scattering.

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A puzzling feature of high T_c cuprate superconductors is the fairly high value of the maximum Δ_0 of the superconducting gap compared to the critical temperature. Indeed it seems to range from 3 to 4 in most experiments, performed mainly on YBCO and on BSCCO [1] . This is to be compared with standard BCS value 1.76 . Since it is widely believed that these compounds are unconventional, with in particular changes of sign for the order parameter, it would seem that this is not much of a problem. However this Δ_0/T_c ratio is surprisingly very stable within all the generalizations of BCS theory which have been put forward for these compounds. Van Hove singularities and more generally any varying density of states raise it at most up to 2 , any reasonable anisotropy [2] gives a result not so much beyond the d-wave value 2.14 and it requires strong coupling effects incompatible with experiments to push it in the experimental range. All these explanations are far from explaining the typical increase by a factor 2 compared to the BCS value, and one may wonder if a more complicated theoretical framework is not necessary in order to account for this ratio.

We show in this paper that this is not the case and that the data can be explained quantitatively to a large extent by a simple theoretical model in the standard framework of mean-field theory. Actually, except for the rather moderate value of the coupling constant we require, all the physical ingredients of our model are known to be present in these compounds, which makes our explanation a very natural one. However we do not apply this claim to the very high values of Δ_0/T_c found recently [3,4] in underdoped BSCCO. We believe that, even if they are clearly related to superconducting properties [5], some additional physics, specific of this regime and this very anisotropic compound, is required to account for such very high results. Our focus is on the more standard values found elsewhere, in other compounds (in particular YBCO) and in optimally and overdoped BSCCO.

The basic idea of our model is the following. As is well known, when a superconductor has an order parameter which changes sign over the Fermi surface, superconductivity tends to be destroyed by anything, like impurities, which scatters electrons between parts of the Fermi surface with opposite signs. If these scattering sources are present at T_c but not at $T = 0$, they will lower the critical temperature but the zero temperature gap will be much less affected. This leads naturally to an increase of the Δ_0/T_c ratio. In order for the number of these scattering sources to be temperature dependent, we have merely to take them as bosons, corresponding to a proper kind of collective modes of our system. Although other kind of fluctuations or modes may be considered, the simplest and most natural choice is phonon scattering. As we will see the typical energy needed for these bosons is in reasonable agreement with the frequencies available for phonons in these compounds.

The idea of explaining a large value of Δ_0/T_c by a decrease of T_c is already present in the literature, but to our knowledge it has not been put to work specifically in the case of d-wave superconductors. It is actually the usual qualitative picture behind the enhanced value of Δ_0/T_c in strongly coupled standard superconductors : the argument is that thermally activated phonons tend to destroy superconductivity and lower T_c while the zero temperature gap is not so affected since there are no real phonons present at T = 0. In the context of high T_c superconductors Lee and Read [6], noticing the strong inelastic scattering experimentally observed, have already proposed qualitatively this kind of mechanism to suggest a lowered T_c. Here we rely specifically on the fact that the order parameter in high T_c superconductors changes sign to obtain an important effect, compatible with experiment. We will more precisely assume the d-wave symmetry, as it is most often done, although our mechanism actually requires only basically that the order parameter takes different signs on the Fermi surface.

In order to explore this kind of explanation and see if it can work quantitatively for high T_c compounds, we take the simplest possible model which retains all the qualitative features of our picture. Specifically we consider a class of models which has already been studied

by Preosti, Kim and Muzikar [7] in the presence of impurity scattering : we mimic a d-wave superconductor by taking an order parameter which takes a constant value Δ_+ on some parts of the Fermi surface and the opposite value $\Delta_- = -\Delta_+$ on the rest of the Fermi surface. We immediately specialize to the situation where the + and − regions have equal weight, as it is the case when they are related by symmetry. We assume that bosons scatter electrons from the + to the − region and vice- versa, and for simplicity we retain only those bosons. We take a simple Einstein spectrum with frequency Ω for these bosons, with coupling constant λ to the electrons. We assume the pairing interaction to have a characteristic energy much higher than T_c and Ω, and take a weak coupling description for the pairing. Therefore we do not make any specific assumption on the pairing mechanism : it may originate from pure Coulomb interaction or from spin fluctuations, or even have a more intricate origin. Again for maximum simplicity we keep only a constant repulsive pairing interaction between the + and the − regions. We do not expect any considerable quantitative changes from all these simplifications, all the more since it is known that the Δ_0/T_c ratio is quite robust.

With all these simplications the Eliashberg equations at temperature T read for our model :

$$\Delta_{\pm,n} Z_{\pm,n} = \pi T \sum_m \Lambda_{n-m} \frac{\Delta_{\mp,m}}{(\omega_m^2 + \Delta_{\mp,m}^2)^{1/2}} \tag{1}$$

$$\omega_n (Z_{\pm,n} - 1) = \pi T \sum_m \lambda_{n-m} \frac{\omega_m}{(\omega_m^2 + \Delta_{\mp,m}^2)^{1/2}} \tag{2}$$

Here $\Delta_{\pm,n}$ and $Z_{\pm,n}$ are the order parameter and the renormalization function at the Matsubara frequency $\omega_n = \pi T(2n+1)$ in the $\pm$ regions. The effective frequency-dependent interaction $\Lambda_n = \lambda_n - k$ contains the pairing interaction k , with a cut-off frequency ω_c and the boson mediated interaction $\lambda_p = \lambda \Omega^2/(\Omega^2 + \omega_p^2)$ with $\omega_p = 2\pi p T$ the boson Matsubara frequency. As mentionned above we have $\omega_c \gg \Omega$ and T_c . When we specialize to d-wave symmetry and insert the corresponding relation $\Delta_{-,n} = -\Delta_{+,n} \equiv \Delta_n$ into these equations, we obtain $Z_{-,n} = Z_{+,n} \equiv Z_n$ and find that Δ_n and Z_n satisfy Eq.(1) and Eq.(2) (with $\Delta_{\pm,n}$ and $Z_{\pm,n}$ replaced by Δ_n and Z_n) provided that we change the sign in front of Λ_n. The resulting equations are just the ones obtained in standard strong coupling theory, except that the roles are reversed between the boson and the Coulomb terms : the boson term is repulsive and the Coulomb one attractive.

We have solved these equations directly both for the change of critical temperature and for the zero temperature gap. However it turns out to be much more convenient to eliminate the pairing interaction and the cut-off in favor of the critical temperature T_c^0 in the absence of boson scattering. This is done by taking explicitely into account that, for $\Omega \ll \omega_n \ll \omega_c$, Δ_n goes to a constant and Z_n goes to 1. Let us first consider the calculation of T_c , where Δ_n gets very small and Z_n takes just its normal state value. We call Δ_∞ this large frequency limit of Δ_n and set $\Delta_n Z_n = \Delta_\infty + d_n$. Since, as can be checked, the pairing term dominates in this range we obtain from Eq.(1) and (2) (after taking into account that Δ_n and Z_n are even functions of ω_n) that Δ_∞ satisfies :

$$\Delta_\infty = 2k\pi T \sum_{m=0}^{\omega_c} \frac{\Delta_\infty + d_m}{\omega_m Z_m} \tag{3}$$

This leads to deal with $S = \pi T \sum d_m/\omega_m Z_m$ where the upper boundary can be taken as infinity since the sum converges. We have also to consider $S' = \pi T \sum 1/\omega_m Z_m$ where we have to keep the cut-off, but this can be expressed in terms of T_c^0 as $S' = S_Z + (1/2)\ln(T_c^0/T) + 1/2k$ with $S_Z = \pi T \sum (1/Z_m - 1)/\omega_m$ where again infinity can be taken as upper boundary. This leads to $\Delta_\infty = -S/[S_Z + (1/2)\ln(T_c^0/T)]$. When this is carried into Eq.(1) this gives the numerically convenient eigenvalue problem :

$$d_n = -\pi T \sum_{m=0}^{\infty} (\lambda_{n-m} + \lambda_{n+m+1}) \frac{\Delta_\infty + d_m}{\omega_m Z_m} \tag{4}$$

which is satisfied when $T = T_c$. Note that a similar procedure could be applied to the standard Eliashberg equations.

We are left with only two parameters, namely the reduced frequency Ω/T_c^0 and the coupling strength λ of the bosons. We have plotted in Fig.1 the ratio T_c/T_c^0, of the critical temperature T_c compared to its value without coupling T_c^0, for various values of the ratio Ω/T_c^0 going from 0.2 to 1. Naturally T_c decreases with increasing λ since boson scattering is pair breaking. High values of Ω/T_c^0 are not of much interest for us since they correspond to a full weak coupling regime, and the ratio Δ/T_c will merely be given by the standard BCS value. Similarly large values of λ lead to a strong decrease of T_c as can be seen in Fig.1 . This produces a large Ω/T_c and leads again to the BCS value for Δ/T_c. On the other hand the result in the low frequency limit $\Omega/T_c^0 \to 0$ is easily obtained. Indeed in this case $\omega_n Z_n = \pi T(2n+1+\lambda)$ and $\lambda_{n-m} + \lambda_{n+m+1} = \lambda \delta_{n,m}$. This leads from Eq.(4) to an explicit expression for the n dependence of d_n and to the result $\ln(T_c^0/T_c) = \psi(\lambda + 1/2) - \psi(1/2)$ where ψ is the digamma function. This is just an Abrikosov-Gorkov result [8], as might have been anticipated since bosons behave as impurities in the $\Omega \to 0$ limit [9]. This analytical result is actually in very good agreement with our numerical calculations for $\Omega = 0.2$. A noticeable feature of Fig.1 is the strong sensitivity of T_c on boson scattering even for moderate coupling strength. Indeed it is severely reduced already for $\lambda \ll 1$. For example the slower decrease of T_c corresponds to the case $\Omega/T_c^0 \to 0$, but even in this case the slope for small λ is $-\pi^2/2$.

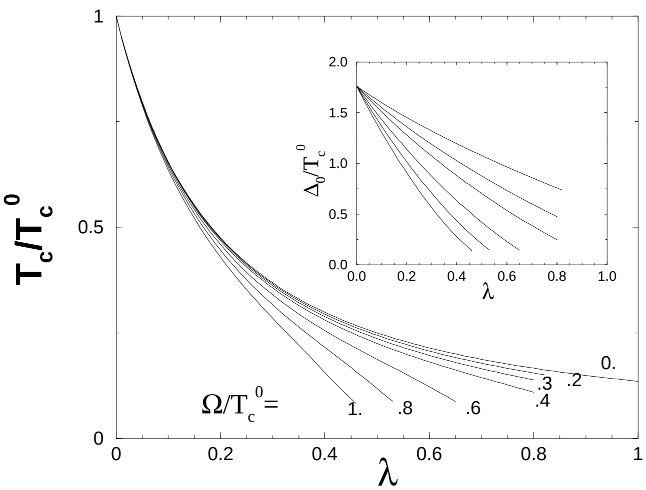

FIG. 1. T_c/T_c^0 as a function of the coupling strength λ for $\Omega/T_c^0 = 0., 0.2, 0.3, 0.4, 0.6, 0.8$ and 1. Insert: Δ_0/T_c^0 as a function of λ, for the same values of Ω/T_c^0 ($\Omega = 0$ omitted).

Let us consider now the calculation of the zero temperature gap, where the situation is somewhat more complicated. In the $T \to 0$ limit Δ_n and Z_n become functions $\Delta(\omega)$ and $Z(\omega)$ of the continuous variable $\omega_n \equiv \omega$. As for the calculation of T_c we set $\Delta(\omega)Z(\omega) = \Delta_\infty + d(\omega)$. In the same way the pairing term dominates in Eq.(1) for large ω which leads to the following equation for Δ_∞ :

$$\Delta_\infty = k \int_0^{\omega_c} d\omega' \frac{\Delta(\omega')}{[\omega'^2 + \Delta^2(\omega')]^{1/2}} \tag{5}$$

where naturally $\Delta(\omega)$ in the right-hand side is expressed in terms of $Z(\omega)$ and $d(\omega)$. For $d(\omega)$ we are left with :

$$d(\omega) = -\frac{1}{2} \int_{-\infty}^{\infty} d\omega' \ \lambda_{\omega-\omega'} \ \frac{\Delta(\omega')}{[\omega'^2 + \Delta^2(\omega')]^{1/2}} \tag{6}$$

with $\lambda_\omega = \lambda\Omega^2/(\Omega^2 + \omega^2)$ and :

$$\omega(Z(\omega) - 1) = \frac{1}{2} \int_{-\infty}^{\infty} d\omega' \ \lambda_{\omega-\omega'} \ \frac{\omega'}{[\omega'^2 + \Delta^2(\omega')]^{1/2}} \tag{7}$$

where we can naturally use the even parity of $\Delta(\omega)$ and $Z(\omega)$. As we have done above for T_c we can use the weak coupling expression for the zero temperature gap $\Delta_{BCS} = 1.76\ T_c^0$ for $\lambda = 0$, obtained from Eq.(5) by setting $\Delta(\omega) = \Delta_\infty = \Delta_{BCS}$, to eliminate the cut-off ω_c and k. This leads to :

$$\ln \frac{\Delta_\infty}{\Delta_{BCS}} = \int_0^{\infty} d\omega \ \frac{\Delta(\omega)/\Delta_\infty}{[\omega^2 + \Delta^2(\omega)]^{1/2}} - \frac{1}{[\omega^2 + \Delta_\infty^2]^{1/2}} \tag{8}$$

This last equation does not provide an explicit expression for Δ_∞ in contrast with what we have for T_c. However this is not in practice a problem, since it can be easily included in the iteration procedure used to solve numerically Eq.(6),(7) and (8). In order to find the gap Δ_0 we still have to continue $\Delta(\omega)$ and $Z(\omega)$ analytically toward the real frequency axis into $\bar{\Delta}(\nu) \equiv \Delta(-i\nu)$ and $\bar{Z}(\nu) \equiv Z(-i\nu)$, and solve $\bar{\Delta}(\Delta_0) = \Delta_0$. This is done by using the explicit expression for this continuation [10]. Note that this analytic continuation lowers noticeably the gap values, compared to the naive evaluation $\Delta_0 = \Delta(0)$.

Just as for T_c , the low boson frequency limit $\Omega \to 0$ is of particular interest. Indeed it leads to a very simple model of strongly interacting fermions with quite non trivial results. Naturally we have in this limit to let λ increase in such a way that $\lambda\Omega$ stays finite otherwise one obtains trivially the BCS result, as it is clear from the equations found below. For this case Eq.(6) and (7) lead to algebraic equations because the lorentzian coming in the integrals gets very narrow. One obtains $Z(\omega) = 1 + \pi\lambda\Omega/2[\omega^2 + \Delta^2(\omega)]^{1/2}$ and $d(\omega) = -\pi\lambda\Omega\Delta(\omega)/2[\omega^2+\Delta^2(\omega)]^{1/2}$, giving for $\Delta(\omega)$ the simple equation :

$$\Delta(\omega) = \Delta_\infty - \pi\lambda\Omega \frac{\Delta(\omega)}{\sqrt{\omega^2 + \Delta^2(\omega)}} \tag{9}$$

This equation (a fourth order equation) can be solved analytically and is very simple to solve numerically. The analytical continuation is merely obtained by replacing ω^2 by $-\nu^2$ in Eq.(9). However one can see easily that the equation $\bar{\Delta}(\nu)/\Delta_\infty = 1 - K\bar{\Delta}(\nu)/[-\nu^2 + \bar{\Delta}^2(\nu)]^{1/2}$, where $K = \pi\lambda\Omega/\Delta_\infty$, has no purely real solution when ν/Δ_∞ becomes larger than $\nu_0/\Delta_\infty = (1 - K^{2/3})^{3/2}$, corresponding to a gap $\Delta_0 = \bar{\Delta}(\nu_0) = \Delta_\infty(1 - K^{2/3})$. Indeed, beyond this point, $\bar{\Delta}(\nu)$ gets complex and the density of states is no longer zero. It is quite interesting to note that, in this limit, this nonzero density of states occurs before the equality $\bar{\Delta}(\Delta_0) = \Delta_0$ is reached. To be complete we have to find the value of Δ_∞ in this limiting situation. The integral in the defining Eq.(8) can actually be performed analytically (essentially by taking $\Delta(\omega)$ as the variable) and is merely equal to $\pi K/4$. Then Δ_∞ is obtained as the solution of the simple transcendental equation $\Delta_\infty/\Delta_{BCS} = \exp(-\pi^2\lambda\Omega/4\Delta_\infty)$. Note that this equation has always a single solution in the physical range $K < 1$.

Coming back to our problem, we have, for $\Omega/T_c^0 = 0.2$ and a varying coupling strength λ, compared the result obtained for Δ_∞ in the limiting situation we have just considered with the general calculation we have performed for any Ω/T_c^0. The agreement is quite good. From this it would be tempting to conclude that, for small Ω/T_c^0, we can also conveniently extract the gap itself from this analytical solution. This is unfortunately not true : a good agreement for imaginary frequencies does not imply that the analytical continuations to the real frequency axis agree quite closely, since this analytical continuation is very sensitive to small differences as it is well known. And indeed in our case there is a sizeable difference between the gaps obtained by the two methods. The results of our calculations for the zero temperature

gap are displayed in the insert of Fig.1. They show that, even for small λ, Δ_0 is quite sensitive to boson scattering, although the effect is not as strong as for T_c. We note in particular that the simple expectation that the gap would be essentially unchanged at $T = 0$ because no bosons are present is not correct.

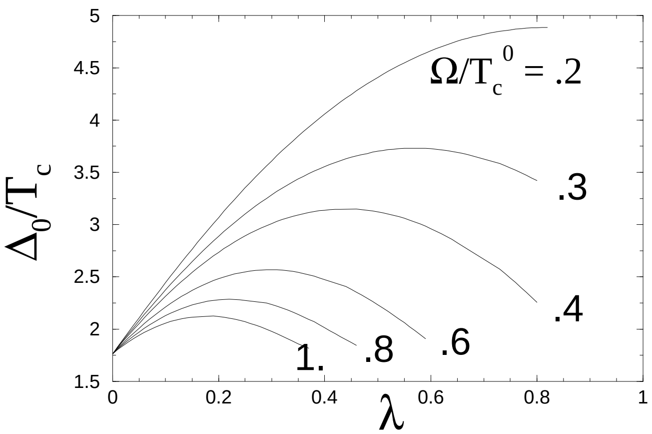

FIG. 2. Ratio of the gap over the critical temperature Δ_0/T_c as a function of the coupling strength λ, for fixed values of $\Omega/T_c^0 = 0.2, 0.3, 0.4, 0.6, 0.8, 1$.

Finally our results for the ratio Δ_0/T_c are shown in Fig.2 for the interesting range of values for the parameter Ω/T_c^0. We note first that, for $\Omega/T_c^0 = 1$, the result does not depart much from the BCS result. Naturally this is even more so for higher values of Ω/T_c^0 for which the results are not displayed. In the same way we find as expected that, for large values of λ, Δ_0/T_c decreases toward the BCS value. Because this is of little interest for our purpose, we have not explored further this regime where numerical calculations get more difficult since one has to deal with very different energy scales. The most interesting feature of our results is naturally the maximum obtained for Δ_0/T_c at intermediate coupling strength. This maximum increases with decreasing Ω/T_c^0 while the λ corresponding to the maximum increases at the same time. In particular for $\Omega/T_c^0 = 0.2$ we find Δ_0/T_c close to 5. Clearly this trend continues as Ω goes to zero. Indeed as it is clear from above, the gap is independent of λ in this limit whereas we have seen that T_c decreases toward zero. Therefore we can in principle obtain a ratio Δ_0/T_c as high as we like. However this would correspond to extreme parameter values.

On the other hand we find among our results a range which is quite compatible with experiments. Indeed for $\Omega/T_c^0 = 0.4$ we obtain a broad maximum for $\lambda \approx .4$ with $\Delta_0/T_c \approx 3.2$. This fairly small value of λ is quite reasonable. The value of Δ_0/T_c is already quite consistent with experimental data, all the more if we take into account that anisotropy of the order parameter is likely to raise Δ_0/T_c by itself, as it does for d-wave in weak coupling where this ratio is raised by 20 %. To be more specific, for $\Omega/T_c^0 = 0.4$, we find $\Delta_0/T_c \geq 3.1$ for $0.36 \leq \lambda \leq 0.52$. For a typical value of $T_c = 90$ K , we find that the range of boson frequency goes from 115 K to 170 K. For $\Omega/T_c^0 = 0.3$ we obtain correspondingly $\Delta_0/T_c \geq 3.6$ for $0.42 \leq \lambda \leq 0.73$, with Ω ranging between 100 K to 170 K. This is a frequency range where an important weight for phonons is known to exist in these compounds. Therefore, at least for optimally doped or overdoped compounds, our explanation for the high value of Δ_0/T_c is completely coherent with experiment, which is quite satisfactory. For markedly underdoped compounds the general situation is no so clear and it is likely that the very high values observed in this case require an additional physical source which might for example be disorder.

However a very striking feature of our interpretation is that it requires a fairly high value of T_c^0, that is the critical temperature without bosons, ranging from 290 K to 420 K for $\Omega/T_c^0 = 0.4$ and from 330 K to 560 K for $\Omega/T_c^0 = 0.3$. Naturally it would be quite desirable to check experimentally this physical aspect of our model. One possible way would be to send a flux of phonons with the proper frequency to see if T_c is affected as expected (these phonons could be generated themselves by tunnel junctions). Another much more interesting, though speculative, possibility is to try to raise T_c toward T_c^0 under static conditions. This could be done through a shift of the phonon spectrum, for example by applying high pressure in order to lower the number of phonons which participate in the decrease of T_c. Actually it is known that, for Hg compounds, T_c increases with pressure, which is compatible with our model. A test would be to measure also Δ_0 under pressure and check that it is less sensitive to pressure than T_c. This would be a clear indication that one can hope to raise T_c even further by modification of the phonon spectrum. It is also important to keep in mind that it is often possible to obtain effectively an increase of pressure by proper chemical substitution in the compound. Therefore an understanding of the effect of pressure would open the way to a possible chemical increase of T_c. Finally it is tempting to believe that the pseudogap observed above T_c in underdoped compounds might be related to T_c^0 and could be obtained by treating our model beyond mean-field theory.

In conclusion we have shown that the adverse effect on d-wave superconductors of boson scattering between regions with opposite sign of the order parameter provide a simple and natural explanation for the high values of Δ_0/T_c observed experimentally.

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